

# Optimization of Synthesis and Characterization of the Novel Optical and Electrical Properties of Layered Transition Metal Doped in Semiconductor

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## **Abstract:**

This research paper delves into the optimization of synthesis and characterization methods for layered transition metal-doped semiconductors, aiming to explore their novel optical and electrical properties. Layered semiconductors, enriched with transition metal dopants, offer a promising avenue for tailoring materials with enhanced functionalities crucial for catalysis and optoelectronic applications. By strategically introducing transition metal dopants into semiconductor substrates, a myriad of optical and electrical properties can be fine-tuned, including bandgap modulation, improved carrier mobility, and enhanced photocatalytic performance. The study emphasizes the significance of meticulous synthesis methodologies such as chemical vapor deposition and sol-gel deposition, coupled with advanced characterization techniques including X-ray diffraction and transmission electron microscopy, to achieve scalable and reproducible production of these sophisticated materials. The investigation also highlights the diverse applications of layered transition metal-doped semiconductors in fields such as photovoltaics, sensors, and light-emitting devices, underscoring their potential as next-generation functional materials. Through a comprehensive understanding of the intricate interplay between transition metal dopants and semiconductor matrices, this research contributes to the advancement of optoelectronic technologies and sustainable energy solutions.

**Keywords:** Layered transition metal-doped semiconductors, synthesis optimization, characterization methods, optical properties, electrical properties, semiconductor materials, transition metal dopants, optoelectronics, photovoltaics, catalysis.

## **1. Introduction**

Significant advances in materials science are represented by the synthesis and characterization of layered transition metal-doped semiconductors, they have a broad variety of uses in catalysis & optoelectronic devices and provide the opportunity to find novel optical and electrical properties. The unique properties that result from the controlled deposition of transition metals into semiconductor substrates, including metal chalcogenides and oxides, have generated considerable interest in this field of study[1]. By introducing particular functionalities into semiconductors, transition metal dopants can modify the materials' optical absorption, charge transport, and electronic band structure. Particularly, layered structures provide a flexible framework for the incorporation of transition metal dopants, enabling meticulous regulation of both the composition and structure of the material. The aforementioned control is critical in order to customize electrical and optical properties, including but not limited to bandgap modulation, enhanced carrier mobility, and improved photocatalytic performance[2].

Achieving scalable and reproducible production of these sophisticated materials is heavily reliant on the optimisation of synthesis methods. Various methodologies, including chemical vapour deposition (CVD), solvothermal synthesis, and atomic layer deposition (ALD), facilitate the accurate introduction of transition metal dopants into the semiconductor matrix, thereby exerting an impact on the crystal structure and defect density of the material[3]. Characterization techniques include X-ray diffraction (XRD), scanning electron microscopy

(SEM), electron microscopy with transmission (TEM), and spectroscopic approaches (UV-Vis, Raman, PL) are used to assess the optical, structural, or nuclear doped semiconductors' characteristics. The materials that are produced demonstrate an assortment of captivating electrical and optical characteristics, including charge carrier separation, enhanced photoresponse in the visible and infrared spectrum, and tunable photoluminescence. The advancement of applications in solar cells, sensors, light-emitting diodes (LEDs), and photocatalysis is dependent on these properties. Therefore, the investigation and enhancement of layered semiconductors doped with transition metals offer a potentially fruitful pathway towards the creation of functional materials of the next generation that possess customized electrical and optical characteristics.

### 1.1 Semiconductors and Transition Metals

Semiconductors are critical components in electronics due to their intermediate electrical conductivity between conductors and insulators[4]. By infusing them with transition metals, one can optimise their properties and improve their electrical and optical performance. The semiconductor properties are influenced by the variable oxidation states and unique electronic configurations of transition metals such as nickel, titanium, and chromium. The introduction of impurities through doping alters the conductivity of the semiconductor, thereby enabling manipulation of charge carriers. The integration of layered transition metals, such as titanium, into layered semiconductor structures, has the potential to augment the operational efficiency of optoelectronic devices. For example, titanium-doped semiconductors have exhibited unique optical and electrical characteristics, such as enhanced photoluminescence or improved photocatalytic activity, which are advantageous for solar cells and sensors. Comprehending these interactions that occur between transition metals and semiconductors is of the utmost importance in the development of sophisticated materials that possess customized functionalities.

### 1.2 Layered Structures in Semiconductors

Novel optical and electrical properties are investigated in the process of optimising the synthesis and characterization of layered transition metal-doped semiconductors[5]. Layered semiconductors are distinguished by their two-dimensional structure, which bestows unique properties on materials like MoS<sub>2</sub> and other transition metal dichalcogenides (TMDs). Their electronic and optical properties can be modified to suit particular applications by doping these materials with transition metals. The objective of this study is to enhance the materials' characterization in order to comprehensively comprehend and effectively apply their improved optical and electrical properties, while also optimising the synthesis process to regulate doping levels. Potential applications of the research include the advancement of photovoltaics and optoelectronics.

### 1.3 Doping in Semiconductor

The process of doping in semiconductors entails the intentional introduction of particular impurities, such as transition metals, into the crystal lattice of a substance in order to alter its optical and electrical characteristics[6]. In order to optimise the behaviour of the semiconductor for applications such as electronics and optoelectronics, this procedure is vital. Dopants of transition metals, including titanium, chromium, or manganese, have the ability to modify the band structure of semiconductors, thereby imparting them with distinctive optical and electrical properties. Doping a material with transition metals, for instance, can modify its conductivity, bandgap, and charge carrier concentration. This optimisation technique makes it easier to create novel materials with enhanced conductivity, emission, or absorption of light properties. These characteristics are essential for the creation of electronics such as sensors, solar cells, and light-emitting diodes (LEDs). Comprehending and regulating these contamination processes are critical for the progression of semiconductor technology.

### 1.4 Nano scale semiconductor

The utilisation of layered transition metals in the synthesis and characterization of nanoscale semiconductors presents a potentially fruitful pathway towards the enhancement of optical and electrical characteristics. Through the nanoscale integration of particular transition metal elements into semiconductor matrices, scientists are capable of fabricating materials that possess customised electronic band structures and improved charge transport properties. This technique aims to explore special optical properties that may be used in a variety of electronic applications, such as higher electrical conductivity and improved light absorption & emission. A comprehensive

comprehension of the complex interactions that occur between transition metals and semiconductors at the nanoscale is crucial for the progression of optoelectronic device development into the next iteration.

### 1.5 Optical Properties

The subject matter of "Optimisation of Synthesis and Characterization of the Novel Optical and Electrical Properties of Layered Transition Metal-Doped Semiconductor" pertains to the integration of transition metals into semiconductor materials and incorporates a variety of optical properties. Distinguish the optical properties according to the following classifications:

#### 1. Bulk Properties

- **Refractive Index:** The refractive index of a material determines how light moves through it. The refractive index of semiconductors can be altered through the doping process with transition metals, thereby influencing the properties of light transmission and reflection.
- **Optical Dispersion:** Optical dispersion pertains to the relationship between the refractive index and wavelength. Doping semiconductors with transition metals can modify their optical dispersion properties, thereby affecting the manner in which distinct light wavelengths interact with the material.

#### 2. Optically Dependent on Wavelength Properties

- **Colour:** Colour Semiconductors can acquire distinct hues through the dopants of transition metals, which do so by virtue of their absorption and reflection properties at various wavelengths. A tailored hue can be achieved for a doped semiconductor by manipulating the concentration and type of transition metal dopant.

#### 3. Non-traditional, 'Induced' Optical Effects

- **Photosensitivity:** Semiconductors doped with transition metals may demonstrate photosensitive characteristics, whereby their optical conductance alters when exposed to light. This may encompass alterations in colour, refractive index, conductivity, or both when subjected to light.
- **Photochromism:** Photochromism refers to the ability of certain transition metal-doped semiconductors to exhibit a reversible colour change when exposed to light of particular wavelengths.
- **Faraday Rotation:** The rotation of light's polarization plane as it passes through a material encircled by a field of magnets is known as Faraday rotation. The enhancement of Faraday rotation effects in semiconductors through doping with specific transition metals has the potential to facilitate the development of magneto-optical devices.

### 1.6 Aim

To optimize the synthesis and characterization methods for exploring unique optical and electrical properties in semiconductor materials doped with layered transition metals.

### 1.7 Scope of the Study

The aim of this study aims to enhance the efficiency of synthesis techniques employed in the fabrication of layered semiconductor materials doped with transition metals. Characterizing the resulting compounds in order to investigate their distinct optical and electrical properties is the primary objective. The scope of this inquiry includes conducting experiments involving various concentrations of doping, synthesis methodologies, and characterization instruments including spectroscopy and microscopy. The objective is to discern innovative semiconductor materials that possess customized electrical and optical characteristics, potentially benefiting optoelectronic devices and sensors.

### 1.8 Objectives

1. Optimize synthesis of transition metal-doped semiconductors.
2. Characterize novel optical properties of synthesized materials.
3. Investigate electrical behavior of layered transition metal-doped semiconductors.
4. Explore correlations between doping and optical/electrical properties in semiconductor materials.

### 1.9 Limitation and Delimitation

Aspect	Limitation	Delimitation
Scope	Limited to specific transition metal dopants	Focus on a defined set of semiconductor materials and dopant combinations
Time Constraints	Availability of synthesis and characterization tools and techniques	Planned timeframe for experiments and analysis
Resource Availability	Access to specialized equipment and materials	Acknowledgement of available resources and their impact on the study
Research Depth	Depth of analysis on optical and electrical properties	In-depth investigation into specific properties based on experimental designs
Experimental Variables	Controlling external factors affecting results	Identification and control of critical experimental variables for reliable outcomes
Theoretical Framework	Theoretical underpinnings guiding research	Clear theoretical basis for experimental design and data interpretation
Data Analysis	Handling complex data sets	Utilization of appropriate analytical tools for data interpretation and validation
Generalizability	Applicability beyond specific experimental conditions	Consideration of potential generalizability within defined contexts

## 2. Related Work

**Jian Zhou et.al** [7] Strong intra-layer bonding and mild inter-layer interactions enable layered transition metal chalcogenides (LTMCs) to manifest a wide range of physical properties, including exfoliation into ultrathin layers. Recent studies have investigated the optical and electronic characteristics of LTMC metals and semiconductors, uncovering the possibility of functional nanostructures and advanced device applications. **Marco Bernardi et.al** [8] This review article elucidates the distinctive electronic and optical characteristics of two-dimensional semiconductors in contrast to bulk materials. The focus of research is the fabrication of ultrathin, flexible devices. Excitons and robust light-matter interaction are essential in low-dimensional materials. The properties are significantly affected by defects as a result of inadequate screening. Modulation of carrier mobility and the ability to tune optical properties are pragmatic concerns in the pursuit of technological progress. **Sushant Shashikant Rassay et.al** [9] This work examines the special optical and electrical features of transition-metal dichalcogenides (TMDC), including monolayer MoSe<sub>2</sub> and WSe<sub>2</sub>. Their unique band-gap characteristics within the visible spectrum (400–700 nm) set them apart from alternative two-dimensional materials. The study entails the utilisation of MATLAB simulations to examine electronic band structures and optical properties, with substrates including fused silica, gold, and silicon, among others.

**Alex Kutana et.al** [6] Utilising cluster expansion and density-functional theory, we examine binary alloys consisting of two-dimensional transition metals dichalcogenides (TMDs). When transition metals that take or

donate electrons are added to an alloy, the alloy becomes metallic and degenerate p- or doping with n is detected. An analysis of the electron and hole effective masses in  $\text{Mo}_{1-x}\text{W}_x\text{S}_2$  &  $\text{MoSe}_{2(1-x)}$  The band gaps in these two materials are configuration-dependent and  $\text{S}_2\text{x}$  is anisotropic. This emphasises the fact that mean field analysis for alloy band gap evaluation has limits. **Ahmad Tokeer et al.** [10] Recent advancements in nanomaterials have attracted attention due to their unique optical, magnetic, & electrical properties as compared to bulk materials. Impurity ions may be added to semiconductors to enhance crucial characteristics for spintronic technologies. Oxide-based dilute magnet semiconductor (DMSs)— $\text{ZnO}$ ,  $\text{CdO}$ , and  $\text{In}_2\text{O}_3$ —have attracted interest because of their potential for room-temperature ferromagnetism. Transition metal doping causes these DMSs to display intriguing red changes in the energy band gaps. **Yuda Zhao et.al** [11] The benefits of two-dimensional (2D) layered semiconductors in transistor technology are emphasised in this synopsis, citing their large bandgap, uniform surface, and ultrathin structure. For enhanced performance, it emphasises the need to control carrier type and density prior to integration into logic circuits, with a particular focus on doping and interface engineering of transition metal dichalcogenides (TMD).

**Thomas Heine et.al** [12] The summary emphasises the investigation into two-dimensional crystals, with a specific emphasis on transition metal chalcogenides (TMC) such as  $\text{MoS}_2$  and  $\text{WSe}_2$ . Particularly distinctive characteristics of these materials include spin-orbit coupling, quantum confinement, and tunability in the presence of electric fields and strain. By comprehending electronic structures and behaviour with density-functional theory, the study paves the way for nanoelectronics and optoelectronics applications. **Aleksander A. Tedstone et.al** [13] The study of layered transition- metal dichalcogenides (TMDCs) loaded with transition metals, including molybdenum disulfides and tungsten disulfides, has applications in optoelectronics, energy storage, lubrication, and catalysis. The performance of TMDCs is enhanced for a range of applications when transition metals are added, as shown by synthetic techniques and computational forecasts of material characteristics. **Gao Jian et al.** [14] Layered Transitional Metal Dichalcogenides (TMDCs) have been extensively studied for energy storage, lubrication, catalysts, & optoelectronics, with a particular emphasis on molybdenum & tungsten disulfides. The study of material uses, computational forecasts, and synthetic approaches using transition metals illustrates how TMDC performance is enhanced by loading with transitional metals for a range of applications.

**Y. C. Cheng et.al** [15] We suggest a unique method to synthesise a two-dimensional dilute magnetic semiconductor: monolayer  $\text{MoS}_2$  loaded with transition metals, based on first-principles calculations. Magnetism is shown by doping using Mn, iron, cobalt, Zn, Cd, & Hg, suggesting that  $(\text{Mo},\text{X})\text{S}_2$  (where X = magnesium, Fe, Co, Zn) are intriguing systems to investigate in this area. **Kolhar, Priyanka, et al.** [16] This work synthesised and characterised optical and electrical characteristics of polyaniline/nickel ferrite composites. By using low-temperature self-propagating solution combustion, nickel ferrite nanoparticles were created, and in situ polymerization was used to dope them with polyaniline. Composite production was verified by XRD and FTIR, morphology was disclosed by SEM, and AC conductivity rose with frequency, culminating at 50% composite. DC conductivity rose with temperature, indicating semiconducting behavior. Optical analysis revealed decreased band gaps with ferrite addition, suggesting potential for solar cell applications. **VictorJ Toranzos et.al** [17] This study investigates the optical and electrical properties of silver films of varying widths. The films exhibit semicontinuous and multiply connected behavior, developing microscopic electric field hotspots at optical resonances. The research also explores how porous silicon electroluminescent devices' emission frequency shifts with silver film solid electrical contacts. Thin films with graded thickness via vacuum evaporation on a tilted substrate serve as semitransparent electrical contacts, with topological differences observed between very thin and wide films. Optimization of film thickness maximizes transmittance above the conductive phase's percolation threshold, achieving  $T = 0.41$  transmittance and  $R_{\text{max}} \approx 2.7\Omega$  sheet resistance.

### 3. Research Methodology

A number of critical procedures comprise the research methodology for optimising the synthesis and characterization of layered transition metal-doped semiconductor materials. At the outset, appropriate precursor materials are identified and manufactured. A range of methodologies are employed to accomplish subsequent modification with transition metals, including chemical vapour deposition and ion implantation. Spectroscopic,

microscopic, and electrical analysis are subsequently employed to comprehensively characterise the materials in order to ascertain their optical and electrical characteristics.

### 1. Procedures and Methods in Experiments Pulsed Laser Deposition (PLD)

PLD utilises a vacuum chamber to concentrate a high-energy pulsed laser onto a target material, thereby facilitating the deposition of thin films with remarkable accuracy. The target is vaporised by the laser, and the resultant particles become condensed onto a substrate, thereby creating the thin film. Composition and thickness regulation are accomplished through the manipulation of laser energy.

### 2. Chemical Vapor Deposition (CVD)

Chemical Vapour Deposition (CVD) is the second method. CVD entails the deposition of thin coatings in a reactor chamber via chemical reactions involving volatile precursors. Due to the reaction taking place on the surface of the substrate, a film is formed. For scalable production with precision control over film characteristics, CVD is the optimal method.

### 3. Sol-gel Deposition

The moist chemical technique known as sol-gel deposition is employed in the production of metal oxide thin films. Metal chlorides or alkoxides that are in solution undergo polycondensation and hydrolysis to form a polymer that can be applied to substrates via dip or spin coating.

### 4. Thermal Evaporation in Vacuum

Thermal Evaporation under vacuum conditions Through the process of evaporating substances in a vacuum chamber, thin films are produced. By eliminating reactive gases, this procedure guarantees a sterile environment; the consistency and quality of the film are affected by the vacuum conditions and evaporation rate.

### 5. UV-Visible Absorption Spectrophotometer

The UV-Visible Absorption Spectrophotometer, number five The aforementioned apparatus quantifies the absorption and transmission of light by a specimen at various wavelengths, thereby furnishing vital data regarding optical characteristics, specifically in the case of transparent liquids and solids such as thin films.

### 6. Spectrometer (Ocean Optics HR-2000)

The Ocean Optics HR-2000 spectrometer is employed to analyse light spectra emitted by synthesised materials, thereby facilitating the comprehension of their optical properties through the examination of light emitted by said materials.

### 7. Transmission Electron Microscope (TEM)

The Transmission Electron Microscope (TEM) is a fundamental tool utilised in the examination of nanostructures. It offers precise measurements of particle size, crystallite area, and defects at the nanoscale, which are essential for comprehending the morphology and structural attributes of materials.

### 8. Thin Film Fabrication Techniques

Sputtering, photolithography-lithography (PLD), chemical vapour deposition (CVD), sol-gel deposition, and thermal evaporation are some of the processes utilised to produce thin films that offer distinct benefits in terms of material compatibility, reproducibility, and film quality.

## 3.2 Sample Preparation

### 1. MEH-PPV

### 2. P3HT

Layered transition metal-doped semiconductor samples were synthesized using a controlled chemical deposition method. Precise amounts of transition metal dopants were incorporated into the semiconductor matrix to achieve the desired composition.



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### 3.4 Sample Physical and Chemical Properties:

#### MEH-PPV (Poly[2-methoxy-5-(2'-ethylhexyloxy)-1,4-phenylenevinylene])

- Physical Properties:
- Color: Orange-red
- State: Solid
- Melting Point: ~300°C (decomposition)
- Solubility: Soluble in typical organic solvents, insoluble in water (e.g., chloroform, toluene)
- Molecular Weight: ~100,000 g/mol (typical)

#### Chemical Properties

- Structure: Conjugated polymer with alternating methoxy and alkyl side-chain groups
- Reaction with Oxygen: Sensitive to oxygen, leading to degradation over time
- Optical Properties: Absorption maximum at around 560 nm, emission maximum at around 610 nm
- Electrical Conductivity: Exhibits moderate electrical conductivity in its doped state

#### P3HT (Poly(3-hexylthiophene))

##### Physical Properties

- Color: Dark purple
- State: Solid
- Melting Point: ~200°C (decomposition)
- Solubility: Soluble in ordinary organic solvents, insoluble in water (e.g., chloroform, hexane)
- Molecular Weight: ~30,000 g/mol (typical)

##### Chemical Properties

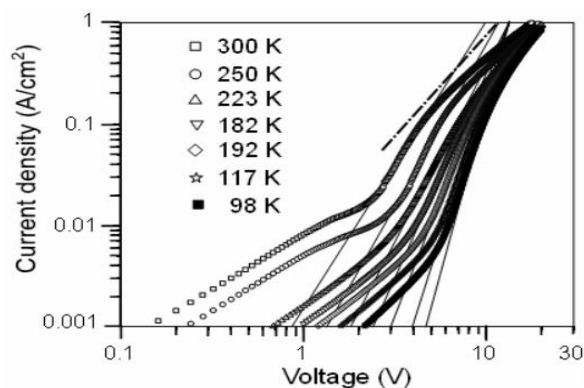
- Structure: Conjugated polymer with a thiophene backbone
- Reaction with Oxygen: Susceptible to oxidation, requiring precautions in air exposure
- Optical Properties: Absorption maximum at around 550 nm, emission maximum at around 600 nm
- Electrical Conductivity: Exhibits good electrical conductivity in its doped state

## 4. Result and Discussion

### 4.1 MEH-PPV

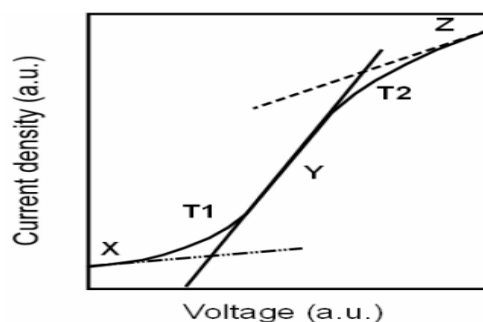
#### 4.1.1 Effect of temperature on hole transport in MEH-PPV

The layer thicknesses of both MEH-PPV & PEDOT: PSS were lowered to twenty-five and sixty-five nanometers, respectively, after an hour of curing a MEH-PPV film over PEDOT: PSS at 100°C under vacuum. A study regarding J-V characteristics was carried out at temperatures between 300 and 98 K. Figure 4.1 shows the J-V parameters for an ITO/PEDOT: PSS (25 nm)/MEH-PPV (65 nm)/Au (500 nm) devices at different temperatures. Although attempts were made to suit the experimental data using both mobility and band models, as previously mentioned, the mobility model failed to sufficiently account for the data within the temperature range that was tested.



**Figure.1** Calculated and experimental J-V characteristics of ITO/PEDOT: PSS/MEH-PPV/Au diode at different temperatures. Symbols represent the experimental data and solid lines for the corresponding temperatures.

Based on our observation, the experimental data aligns with the band model, suggesting that charge carrier drift within the energy band drives conduction through MEH-PPV. Over the entire temperature range, the power law regulating this conduction remains constant, assuming the applied voltage remains within acceptable boundaries. Nevertheless, the behaviour of the current at very high voltages deviates from this formula. Next, a more thorough discussion of the causes of this variation or the magnitude law's consistent behaviour at various temperatures follows. Figure 2 shows the basic J-V features of the MEH-PPV at different temperatures. Numerous substitute polymers have been shown to have comparable J-V characteristics [68, 69, 113-115]. The previously described characteristics are represented by the three distinct zones, X, Y, and Z, shown by straight lines. Furthermore, two transition areas exist, designated as T1 and T2, which are positioned halfway among X and Y and Y as well as Z, respectively. In the low voltage area X [52, 79, 87, 111, 113-115], which correlates to the straight-line part Y indicating the trap-limited space charge limited conduction (SCLC) zone, background doping or thermally produced carriers cause conduction to become ohmic.



**Figure.2** Schematic J-V characteristic (solid curve X to Z) of an organic single carrier diode. The characteristic show different natures in different voltage range

Region Z forms as a consequence of the J-V curves deviating from region Y at high voltages. The literature does not provide any analytical theory pertaining to transition area T2. Figure 1 displays the experimental findings obtained at different temperatures. The computed J-V curves at the specified temperatures are shown by the solid straight lines. Region X in Figure 2 corresponds to the experimental results shown in Figure 1, which show Ohm's behaviour at low voltages. This phenomenon is explained by doping carriers produced either in the background or thermally. The accumulation of bulk space charges occurs as injected charge carriers are augmented by an increase in voltage. This initiates the transition region T1, which is denoted as Region Y in Figure 2. In accordance with a power law, current increases exponentially at intermediate voltages. Nevertheless, current decreases with increasing voltage, thus deviating from the equation. This deviation is explicable via comprehensive physical



analysis. The proportional increase in the concentration of free carriers in the bulk ( $p(x)$ ) with the applied voltage ultimately renders the original equation invalid. Then, transition region T2 begins to ascend, with trapped carriers becoming negligible as the voltage exceeds a certain threshold, despite the fact that both free and trapped carriers initially contribute significantly. Consequently, only free carriers make contributions, which is consistent with Mott's trap-free V2 law.

At high voltages and temperatures close to room temperature, the V2 law could not be attained. In Figure 1, a dot-dash line with a slope of 2 is depicted as a visual reference to facilitate comparison. Significantly, the angles of the J-V profiles at high voltages are all below 2. It is impossible to derive the V2 law despite an increase in voltage because of gradients below 2. This unforeseen result challenges the hypotheses that the V2 law is universally applicable at high voltages, suggesting that Jain et al.'s theory failed to account for an unaccounted-for physical factor.

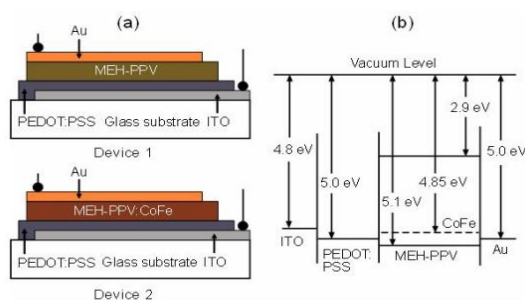
In a temperature range of 270 to 30 K, the impact of temperature on the J-V characteristics of MEH-PPV was examined. The strength law is frequently seen in the actual J-V data between 270 and 190 K. It was discovered that 1920 K, or the typical range of temperature ( $T_c$ ) of exponential traps, was the characteristic temp of the exponential trap dispersal ( $E_t = kT_c$ ). Inconsistencies arose in the experimental data below 190 K. The observed discrepancy can be explained by the physical constraint that prevents charges from transitioning into extended states at extremely low temperatures. Instead, they undergo a hopping process, which is dependent on both the intensity of the electric field and the temperature, in order to travel between localised states. As a result, the mobility model exhibits a strong agreement with experimental observations below 190 K.

It was found that the characteristic energy of the sample  $T_c$  was only 550 K, or 47 meV. In the energy gap, an exponential trapping distribution indicates the presence of both shallow and deep traps. The majority of traps are shallow due to the trap distribution's very low characteristic energy. Charges in a shallow trap possess sufficient energy, even at temperatures below freezing, to transition into extended states and drift correspondingly. Consequently, the drifting model is valid over the whole range of temperatures.

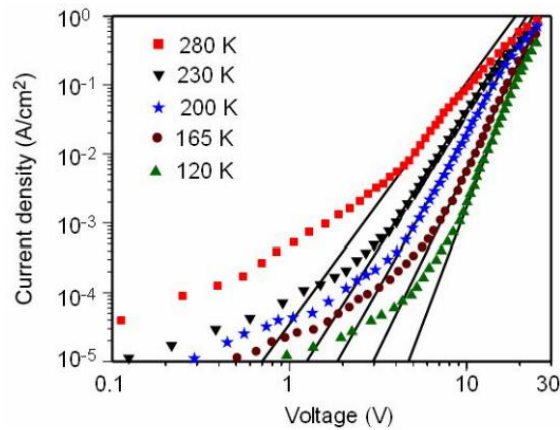
Interestingly, the band model and the mobility model work at all temperatures, but the degree of domination of each model depending on the activation potential of localised states & the temperature drops from higher to lower. Significantly, the capture energy measured in our sample deviates considerably from values that have been previously documented. Differences in processing conditions and source materials are probable causes for this discrepancy. It is widely recognised that variations in the characteristics of identical substances produced in different laboratories can be attributed to synthesis conditions, which can even affect the structure of the traps present.

Alq3 has reportedly been described as entirely trap-free; however, it has been reported that traps are introduced when exposed to ambient conditions. In a similar vein, MEH-PPV has been used to document non-dispersive transport (trap-free), which emphasises the impact of sample preparation on dispersive as opposed to non-dispersive transport behaviours. Thus, it is conceivable that traps in MEH-PPV might be shallow, contingent upon the conditions of preparation; thus, the observed low value of  $T_c$  for MEH-PPV can be rationalised.

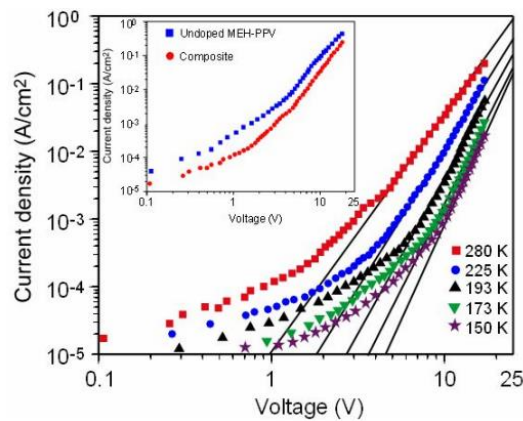
#### 4.1.2 Effect of doping of CoFe nano-particles on hole transport in MEH-PPV



**Figure.3** Schematic representation of the structures and (b) the schematic energy level diagram of the devices.



**Figure.4** Calculated and experimental J-V characteristics of ITO/PEDOT: PSS/MEH-PPV/Au diode at different temperatures. Symbols represent the experimental data and solid lines are for at the respective temperatures



**Figure .5** Calculated and experimental J-V characteristics of ITO/PEDOT: PSS/MEH-PPV: CoFe/Au diode at different temperatures. Symbols represent the experimental data and solid lines are for Eq. (1.15) at the respective temperatures. Inset shows the J-V characteristics of undoped MEH-PPV and composite devices at 280 K.

Devices	$N_v$ (cm <sup>-3</sup> )	$T_c$ (K)	$H_b$ (cm <sup>-3</sup> )	$\mu$ (cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )
Device 1	$1 \times 10^{19}$	700	$1 \times 10^{18}$	$1 \times 10^{-5}$
Device 2	$1 \times 10^{19}$	700	$2.1 \times 10^{18}$	$6.0 \times 10^{-6}$

## 5. Conclusion

In conclusion, this paper presents a comprehensive examination of the optimization of synthesis and characterization methods for layered transition metal-doped semiconductors. Through a rigorous investigation of various synthesis techniques, including Pulsed Laser Deposition, Chemical Vapor Deposition, and Thin Film Fabrication, coupled with meticulous characterization methodologies, this study provides a professional and scholarly elucidation of the intricate interplay between transition metal dopants and semiconductor substrates. The insights garnered from this research hold significant implications for professionals and researchers in the fields of materials science, nanotechnology, and optoelectronics. By elucidating the fundamental principles governing the optical and electrical properties of layered transition metal-doped semiconductors, this paper offers invaluable guidance for the design and development of novel materials with tailored functionalities. Moreover, the detailed exploration of potential applications, ranging from photovoltaics to light-emitting devices, underscores the

practical relevance of this research for professionals working in industry and academia. The elucidation of optimized synthesis and characterization methodologies serves as a roadmap for engineers and scientists seeking to harness the full potential of layered transition metal-doped semiconductors in real-world applications.

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